ACCES: AUTONOMOUS CHARACTERISATION AND CALIBRATION USING EVOLUTIONARY SIMULATION

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The discrete element method (DEM) is a powerful simulation technique that is capable of numerically modelling the behaviour of complex granular media, being used to better understand and optimise the internal dynamics of a large number of systems and multiphase flow processes in both academic fields and industrial sectors, from fundamental research into contact mechanics to improving plant-scale reactors [Rosato and Windows-Yule, 2020]. DEM can offer exceptional accuracy through its lack of approximations over meshes and, if correctly calibrated, simulations can provide results with quantitative precision. It is this "if", however, that also represents DEM's biggest drawback: without choosing appropriate contact models and carefully calibrating multiple DEM parameters, the simulation outputs simply cannot be trusted. This calibration is a time-consuming process, typically involving the measurement of diverse particle properties including size, density, restitution and friction coefficients and, for purely "virtual" parameters such as the cohesive energy density, a great deal of experimentation [Luding, 2008].

To automate DEM calibration against experimental measurements, we have developed ACCES – Autonomous Characterisation and Calibration using Evolutionary Simulation. ACCES enables a researcher to calibrate virtually any DEM parameters against a user-defined cost function, quantifying and subsequently minimising the disparity between the simulated system and the experimental reality using state-of-the-art evolutionary strategies – in essence, autonomously 'learning' the physical properties of the particles within the system, without the need for human input. This cost function is completely general, allowing ACCES to calibrate DEM against measurements as simple as photographed occupancy plots, or complex system properties captured through e.g. Lagrangian particle tracking in multiphase flow processes. The algorithm itself is completely DEM engine-agnostic; it was implemented in an open-source Python library, providing an interface that is easy to use, but powerful enough to automatically parallelise arbitrary user scripts through code inspection and metaprogramming.

ACCES has been used successfully from laptop-scale shared- memory machines to multi-node supercomputing clusters, namely BlueBEAR, running hundreds of simulations simultaneously over numerous projects and types of simulation software. These projects and their BlueBEAR usage will be discussed in the oral presentation, showcasing how BEAR has been vital in for industrially relevant projects as well as pure academic research.

References

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